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Computer simulations to study the effects of explosive and confinement properties on the deflagration-to-detonation transition (DDT)

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Abstract. We have augmented the HERMES model (High Explosive Response to MEchanical Stimulus) by adding a modified CREST (Computational Reaction Evolution dependent on Entropy (S) and Time) detonation model. We have applied the combined model in ALE3D to simulate DDT in an experimental configuration comprising an explosive confined in a tube and ignited at one end. We assess the quantitative effects of explosive properties and of tube geometry and strength on the location of the detonation transition. For a fixed porosity, we find that the specific surface area of the explosive particles, in combination with the explosive's pressure-dependent burn rate, have strong influence on the transition to detonation. The run-to-detonation properties of the explosive powder (given by the Pop-plot) also have strong effect. In our simulations, the speed of the ignition front has somewhat less effect on the transition. The ignition front is caused by hot product gas moving through the permeable bed of explosive particles. In our single-velocity, multi-species approximation, we specify the ignition front speed as an input parameter. The results of our simulations help us identify the independent experiments that must be performed and analysed before a model for DDT can be validated.

1. Introduction

The HERMES model [1, 2] was developed to describe the behaviour of solid explosives and propellants in postulated accidents that do not produce prompt detonations. We have embedded the model in the computer simulation programs LS-DYNA [3] and ALE3D [4], and performed simulations of a number of different explosives and propellants in various experimental test vehicles. Those tests that ignited resulted in more-or-less violent reactions that never detonated [1].

HERMES included a constitutive description of flow stress as a function of strain, strain-rate, pressure, ambient temperature, and porosity. Surface area and porosity increased with shear deformation, and porosity decreased with compaction. It included an ignition criterion, the subsonic propagation of an ignition front through damaged material, and the build-up of gas products (and as a result, pressure) as the burn progressed. In this way it described deformation, ignition, and post-ignition behaviour in the framework of multi-species but single velocity treatment that enforced pressure but not temperature equilibrium between reactant and product.

Depending on the severity of the mechanical insult and/or confinement strength and/or explosive mass, we wished to know whether igniting a deflagration could transition to a detonation. To this end, we recently incorporated a subset of the CREST [5] detonation model in HERMES. We chose

CREST, rather than a pressure-based ignition and growth model [6], because CREST intrinsically distinguishes a shock pressure from the subsonic rise in pressure to the same value, which occurs during deflagration. In HERMES, the mass fraction of reactant converted to product increases by the sum of the reaction rate calculated from the CREST detonation model and the reaction rate calculated from the original HERMES formulation for the burn-up of broken explosive.

Applying multi-phase, multi-velocity or multi-phase, single velocity treatments to describe DDT is not new [7-9]. What we present here is an extensive parameter study of the many factors that influence the location of the detonation transition that have not, in general, been highlighted previously. As a result, we observe that results of additional experimental tests, not customarily reported, need to be known before a model can be validated. Our model has not yet been validated.

We present here the results of applying the HERMES model in ALE3D to DDT test geometry, using HMX explosive at 86% of the crystal density (86% TMD). The calculational geometry is an axisymmetric approximation of the High Confinement Apparatus used by Sandusky [10], which confines the explosive in a 340 mm long mild steel tube, with 25 mm inner diameter and 76 mm outer diameter, and 25 mm thick endplates. In our simulations we have removed the PTFE disk located at the far endplate and replaced it with additional explosive. For our baseline calculations the particles are spheres of diameter 1.5 mm, which roughly correspond to the size of moulding powder beads of several different plastic bonded explosives. The particle size distribution of the beads used in Sandusky's experiments is just now being measured. In our simulations we ignite a 1 mm thick pancake of explosive that fills the base of the tube. This permits our mesh resolution study to refer to the same initial conditions.

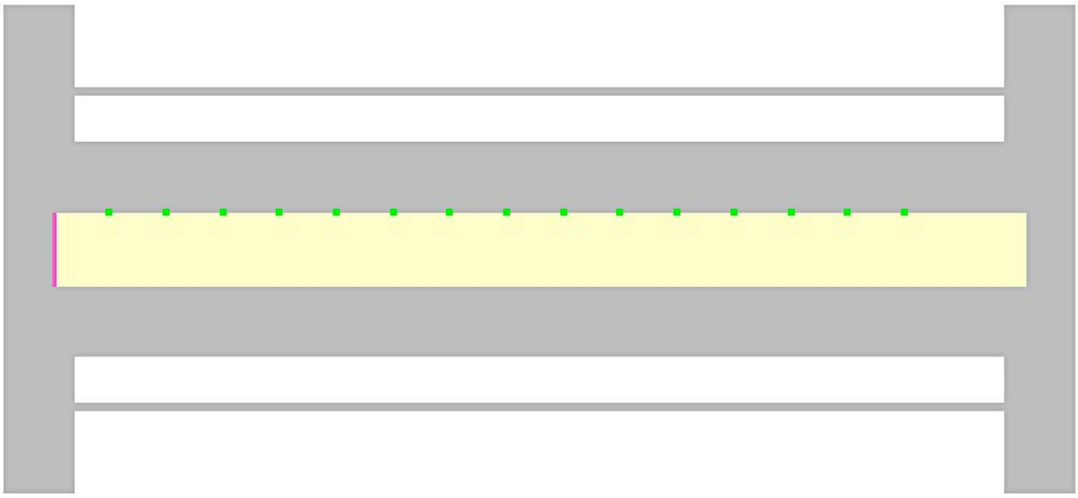

Figure 1. Axisymmetric approximation of the DDT apparatus of Sandusky [10]. The thin outer cylinder is an axisymmetric representation of the 4 bolts used in the experiment. The explosive fill (yellow) is 340 mm long. The green dots represent every other computational gauge location, at which the stress component normal to the tube wall is recorded. The thin (red) disk at the left side is the location of the volume of material ignited at time zero.

2. Locating the transition to detonation

We discovered that there is the potential for significant ambiguity when simplifying a continuous transition to full detonation by reporting only a single point location. In our study we recorded the radial stress in the finite element of the steel tube adjacent to the explosive at 10 mm intervals along the axis of the tube. This corresponds roughly to the output of piezoelectric pins mounted in the tube wall. We found, however, that we obtained significantly different arrival times during the build-up to detonation, depending on the stress value we chose as the triggering threshold. With a very low amplitude (< 10 MPa) set point, the gauges nearest the ignition plane reported a velocity that was equal to the pre-selected velocity of the ignition front moving through the powder bed. As pressure builds, the bed compresses with a propagation velocity that out-runs the ignition front. The velocity of propagation, of course, depends on the details of dynamic compaction of the bed. HERMES uses the P-α model of Herrmann [11] but the parameters are based on compaction experiments on a different explosive formulation. Eventually a shock is formed that results in a significantly enhanced local burn rate according to the CREST model. The shock then grows in amplitude to produce a detonation transition similar to the one that occurs in shock to detonation transition (SDT) experiments on porous explosives.

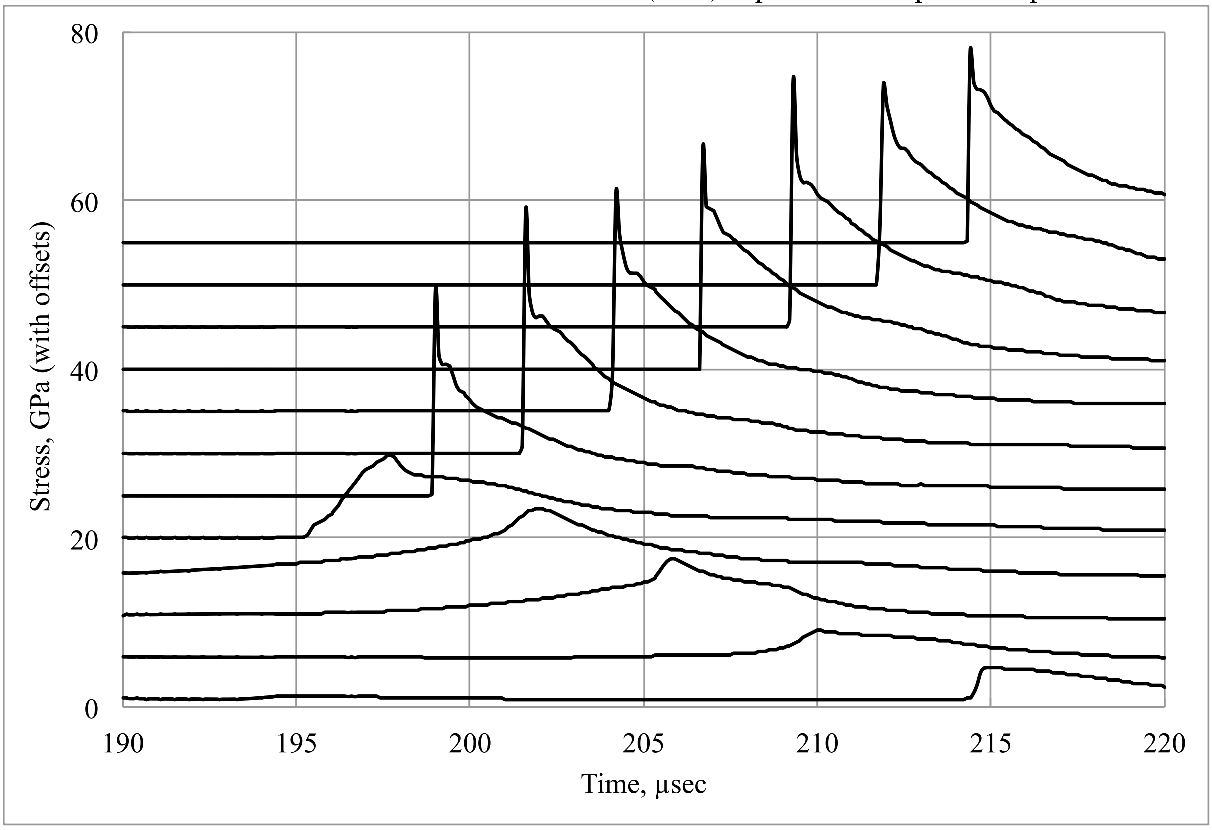

Figure 2. Normal stress histories recorded from every other gauge location. For clarity, each successive history has been displaced by 5 GPa.

For most SDT experiments and computer simulations, the location of the transition (run distance) is taken to be the intersection of two lines tangent to the time-of-arrival vs. distance plot. The first line is tangent to the pre-detonation side shock arrival. It has a slope determined by the propagation velocity of the input shock in the unreacted explosive. The second line (post-detonation side) has a slope determined by the detonation velocity in the (reduced initial density) explosive. The fast rise time of shock waves means that the arrival time is essentially independent of the triggering threshold stress chosen, which is often taken to be about half the shock strength. For DDT experiments and simulations, the input stimulus is weak, and the pre-detonation pressure grows gradually, but with an increasing pressurization rate. As a result, the arrival time of a signal on the pre-detonation side depends strongly on the triggering threshold stress chosen. (See Figure 2 for the gradual pre-detonation pressure rise.) Figure 3 illustrates the sensitivity of the time of arrival to the triggering threshold stress on the pre-detonation side. Since the post-detonation side is a shock wave, the time of arrival is independent of the triggering threshold stress. As a result, we have chosen to take the point where the signal propagation velocity is 95% of the detonation velocity. The pressure is a shock wave, so the time of arrival is independent of the triggering threshold stress. In addition, the pressure is nearly the full detonation pressure, so that the point chosen by this method is similar to what one would infer by looking at the deformation of the tube wall.

In some experiments [12], luminosity is used to infer time of arrival by using a streak camera focused on a long slit in the confining tube wall that is filled with a thin glass plate. We see a similar difference in our calculated arrival times using temperature in the explosive reactant and product mixture measured at locations fixed in space. This corresponds roughly to fibre-optic probes inserted in the tube wall at 10 mm intervals. If the recording instruments were sensitive enough to respond to low temperatures, say 500K, then according to our simulations, the pre-detonation side would record the ignition front velocity. If typical cameras are used, then only relatively high temperatures are recorded, say above 2000K. In that case according to our simulations, retonation would be observed.

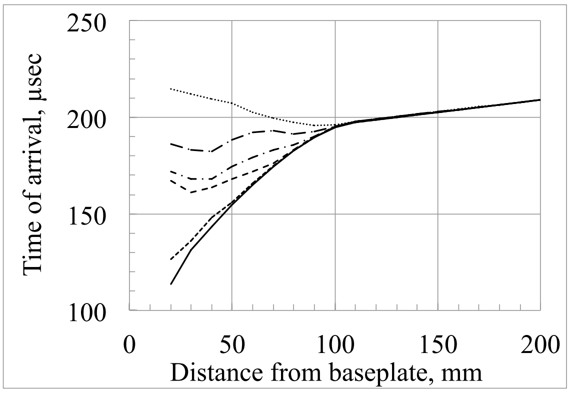

Figure 3. Time of arrival (μsec) as a function of distance (mm) for pressure set points of (top to bottom) 3, 1, 0.5, 0.3, 0.1, and 0.01 GPa. The transition point is 114 mm.

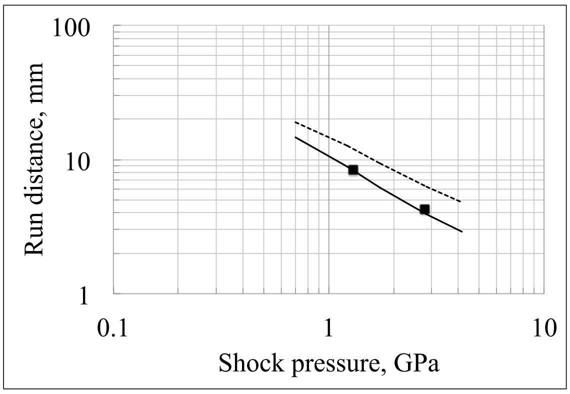

Figure 4. Run distance (mm) as a function of shock pressure GPa) for baseline calculation (solid) and reduced sensitivity calculation (dash). Data points from [15]

3. Results of the simulations

The baseline calculation used 0.2 mm square elements everywhere. The transition point calculated using 0.1 mm elements was also 114 mm, but increased to 116 mm using 0.33 mm elements. The remainder of the simulations used 0.2 mm elements.

Changing the size of the moulding powder beads has a significant effect on the transition point. Our baseline calculation used 1.5 mm diameter beads. The transition point changes from 99 mm for 1 mm beads to 204 mm for 5 mm beads. The laminar burn velocity used in the simulations has similar effect to changing the bead diameter. We used a burn velocity characteristic of HMX explosives that is linear in pressure and takes the value 100 mm/s at a 100 MPa. Measurements of the mass-burning rate of an HMX powder bed are in process.

The confinement has a significant effect on the transition point. The baseline calculation used steel with 350 MPa yield (0.2% offset) and 640 MPa ultimate strengths, which corresponds roughly to 1018 steel. A calculation with half the wall thickness resulted in a transition at 124 mm. Using steel with half the strength (170 MPa yield, 330 MPa ultimate also described as mild steel [13]) had a 124 mm transition as well. Using much stronger alloy steel [14] (1060 MPa yield, 1130 MPa ultimate) gave a 110 mm transition. Many calculations of DDT use a one-dimensional approximation, where no wall expansion is permitted. The transition point in our one-dimensional calculation was 104 mm.

We varied the velocity of the ignition front from 100 to 400 m/s (baseline value 200 m/s) with essentially no effect on the transition location for the baseline 1.5 mm moulding powder beads. In contrast, calculations with 5 mm beads (or equivalently a slower laminar burn rate) showed significant increase from 204 mm to 252 mm when we increased the ignition front velocity to 400 m/s.

The SDT characteristics have significant effect on the calculated transition point. Garcia *et al*. [15] report measurement of the run to detonation in 86% TMD HMX powder. We used that data to obtain parameters for CREST for the calculations. Using CREST parameters that give a run distance about 150% of the baseline calculated at the same shock pressure (figure 4) resulted in a transition point of 144 mm.

The strength of the explosive also has an effect on the transition. The baseline calculation uses compaction strength of 300 MPa and a maximum yield strength of 200 MPa. Reducing both the compaction strength to zero (snowplough model) and the yield strength to zero decreases the transition to 111 mm. For 5 mm beads, the transition decrease was more significant, from 204 to 173 mm.

4. Conclusions

We have conducted an extensive parameter study using the HERMES model to calculate DDT in a typical DDT apparatus. By doing so, we highlight the independent measurements (and simulations) needed to validate a model.

Many DDT experiments were performed as SDT tests, using a moving piston rather than static ignition to start the test. Measurements and simulations of SDT for the powder morphology and starting density are needed for both kinds of tests. The particle size distribution must be measured. The confinement strength must be measured. Descriptors such as "mild steel" or "annealed" are inadequate. From our calculational results, measuring the ignition front velocity is especially important when the mass-burning rate behind that front is small. We speculate that the front velocity will also be important for high porosity tests, where the development of pressure is delayed. The resistance to compaction and compressive strength of the explosive must be measured.

We use a pressure-dependent laminar burn speed based on measurements of low porosity pressed explosive. Although this burn speed is used to infer the particle size distribution in closed bomb tests using small amounts of broken explosive ignited simultaneously, experiments are needed to determine whether this is appropriate for DDT experiments as well, or whether convective burn near the ignited volume will result in an enhanced burn rate.

5. References

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